

Entanglements in Systems with Multiple Degrees of Freedom

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In this letter we present the entanglement properties of the spin-orbital coupling systems with multiple degrees of freedom. After constructing the maximally entangled spin-orbital basis of bipartite, we find that the quantum entanglement length in the noninteracting itinerant Fermion system with spin and orbit is considerably larger than that in the system with only spin. In the $SU(2) \otimes SU(2)$ spin-orbital interacting system, the entanglement, expressed in terms of the spin-orbital correlation functions, clearly manifests the close relationship with the quantum phases in strongly correlated systems; and the entanglement phase diagram of the finite-size systems is in agreement with the magnetic and orbital phase diagram of the infinite systems. The application of the present theory on nucleon systems is suggested.

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The total spin wavefunction of two entangled particles with spin-1/2 can not be expressed as the direct product of the wavefunctions of the two individual particles, and the measurement to the spin of one individual particle inevitably brings out the information of the spin states of the other particle. This property provides wide potential application in quantum computer and quantum teleportation. Entanglement properties in quantum many-particle systems have received great interests in recent years since it is realized that, on the one hand, the entanglement may characterize the quantum correlations between particles [1, 2], or even the quantum phase transitions in some simple models [3, 4, 5, 6]; on the other hand, the realization of quantum computation in solid devices also naturally raises the question, e.g. how these electrons entangle with each other in the presence of strong correlations. Up to date, most of studies are concentrated on the spin entanglement of many-particle systems. While in quantum many-particle systems, besides the spin freedom degree, the particle may possess other degrees of freedom (DOF), such as the orbit, the position and the momentum, etc. Especially in the strongly correlated electronic systems, the orbital DOF is important for the relatively localized 3d or 4f electrons [7]. Little was known about the entanglement properties of the particles with multiple freedom degrees. In this letter we present the entangled properties of strongly correlated particles with multiple DOF. After constructing the maximally entangled states, the Bell basis, of two particles with spin and orbit, we first demonstrate that the quantum entanglement length in itinerant electron system with two DOF becomes significantly larger than that in the system with only spin. In the strongly interacting spin-orbital systems with $SU(2) \otimes SU(2)$ symmetry, the entanglement evolves with the quantum phases, and appears abrupt changes near the critical points of the quantum phase transitions. The entanglement phase diagram highly coincides with the magnetic and orbital phase diagram. Finally we dis-

cuss the possible application of the present theory on the nucleon systems with multiple DOF.

Considering the quarter-filling ($\nu=1/4$) quantum many-particle systems with spin $S=1/2$ and twofold-degenerate orbital DOF, we introduce the pseudospin operator $\hat{\tau}$ to describe the two orbital states: $\hat{\tau} = \sum_{ab} C_a^\dagger \sigma_{ab} C_b$, here σ is the Pauli matrix, and the orbital indices a, b run over 1 and 2. As well known, an entangled state is unfactorizable, and a bipartite with maximally entangled state is completely indivisibility. For a bipartite with two electrons at site A and site B with spin DOF, the Bell basis consists of four states $|\psi_{1,2}^s\rangle_{AB} = (|\uparrow\uparrow\rangle \pm |\downarrow\downarrow\rangle)/\sqrt{2}$, and $|\psi_{3,4}^s\rangle_{AB} = (|\uparrow\downarrow\rangle \pm |\downarrow\uparrow\rangle)/\sqrt{2}$. These Bell states with maximized entanglement are the foundation of quantum information theory and quantum computation [8]. In the presence of both spin and orbital DOF, we find that the possible Bell basis is separated into two independent groups.

(i) The first group is composed of the direct product of the entangled spin and the entangled orbital parts, and each part is a Bell sub-basis, i.e., maximally entangled. The 16 basis wavefunctions in the present situation can be readily constructed: $|\psi^{s\tau}\rangle_{AB} = |\psi^s\rangle^{Bell} \otimes |\psi^\tau\rangle^{Bell}$, where $|\psi^s\rangle^{Bell}$ and $|\psi^\tau\rangle^{Bell}$ represent the spin and orbital Bell states, respectively, e.g.

$$|\psi^{s\tau}\rangle_{1,2} = (|\uparrow\uparrow\rangle \pm |\downarrow\downarrow\rangle) \otimes (|11\rangle \pm |22\rangle) \quad (1)$$

etc. Similar to the spin case, the 16 states in this group are the common eigenstates of the operator set $(\sigma_A^x \sigma_B^x \tau_A^x \tau_B^x, \sigma_A^z \sigma_B^z \tau_A^x \tau_B^x, \sigma_A^x \sigma_B^x \tau_A^z \tau_B^z, \sigma_A^z \sigma_B^z \tau_A^z \tau_B^z)$. One can use these operations to generate the 16 states in this group without difficulty.

(ii) The second group of the Bell basis is consisted of 16 spin-orbital states which are the linear combination of independent spin-orbital parts, e.g.

$$|\phi^{s\tau}\rangle_{1,2} = (|11\rangle^\tau \otimes |\psi_1^s\rangle \pm |22\rangle^\tau \otimes |\psi_2^s\rangle)/\sqrt{2} \quad (2)$$

etc., here $|\psi_i^s\rangle$ is the i -th spin Bell subbasis. We notice that as the candidates for the maximally entangled basis, each group of these basis is orthonormalized and complete set.

In order to justify if these are the maximally entangled states, the degree of entanglement of these states is quantified. For a many-state bipartite, the negativity is a good operational measurement to quantify the entanglement since it is monotonic under the local operation and the classical communication, and it vanishes if two subsystems are not entangled [9]: $\aleph_{A,B} = (||\rho^{TA}|| - 1)/2$, where $||\rho^{TA}||$ is the trace norm of the partial transpose of the density matrix of subsystem A versus to the B and satisfies: $||\rho^{TA}|| = Tr\sqrt{\rho^{TA}(\rho^{TA})^\dagger}$. Interestingly, since spin and orbit are two independent DOF, we could introduce the spin and the orbital sub-entanglements to quantify the entanglement degree of each DOF after trace out the other DOF: $\aleph^{s(\tau)} = (||\rho_{s(\tau)}^{TA}|| - 1)/2$, where $\rho_{s(\tau)} = Tr_{\tau(s)}(\rho)$. We find both of the two groups of the basis have the maximal entanglement with the von Neumann entropy $E_{AB} = 1$ and the negativity $\aleph_{AB} = 1.5$. However the spin and the orbital sub-entanglements of these two subgroups are different: in the first group, the spin or orbital maximal sub-entanglement of each state is $\aleph_{AB}^{s(\tau)} = 0.5$; whileas in the second group, the spin or the orbital sub-entanglement of each state completely vanishes. Such significant difference in the sub-entanglement reflects the distinct character of these two group basis: the former is composed of the independent spin or orbital Bell states, while the latter of spin-orbital indivisible bipartite.

A. Entanglement in Itinerant Fermion Systems

Before investigating the entanglement in the spin-orbital interacting system, we first explore the bipartite entanglement in non-interacting itinerant electron system with spin and orbital DOF. The spin entanglement of two electrons in noninteracting Fermi gas with single spin DOF was known [10, 11, 12]. In the system with only spin, the entanglement vanishes when the spatial separation of two electrons is larger than a characteristic length r_e^0 , $r_e^0 \approx 1.8/k_F^0$, where k_F^0 is the zero-temperature Fermi momentum. In the spin-orbital itinerant electron system, we find that the spin-orbital entanglement length of two electrons becomes considerably large, and the sub-entanglement of the bipartite for individual DOF is zero even in the most entangled spin-orbital states.

At zero temperature in the ground state, the electrons occupy all the levels below the Fermi surface $|\psi_0\rangle = \prod_{s,\tau,|k|\leq k_F} c_{\mathbf{k},s,\tau}^\dagger |0\rangle$, where the Fermi wavevector k_F satisfies $k_F = (3\pi^2 N/2V)^{1/3}$. From the density matrix $\rho_N = |\psi_0\rangle\langle\psi_0|$, the two-particle density matrix ρ_{12} is obtained through tracing over other particles $\rho_{12} = Tr\{\rho_N \phi^+(2')\phi^+(1')\phi(1)\phi(2)\}$ [13], where $1 = (\mathbf{r}_1, \sigma_1, \tau_1)$, \mathbf{r}_1 is the position vector, and the oper-

ator $\phi(1) = 1/\sqrt{V} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{r}_1} c_{\mathbf{k},s,\tau}$. Taking into account the spatial diagonal element, we obtain the reduced two-particle spin-orbital density matrix,

$$\rho_{12} = [\delta_{\sigma_1\tau_1;\sigma'_1\tau'_1} \delta_{\sigma_2\tau_2;\sigma'_2\tau'_2} - f(r)^2 \delta_{\sigma_1\tau_1;\sigma'_2\tau'_2} \delta_{\sigma_2\tau_2;\sigma'_1\tau'_1}] / [16 - 4f(r)^2] \quad (3)$$

where $f(r) = 3(\sin x - x \cos x)/x^3$ with $x = k_F r$. For this mixed-state density matrix, the negativity is larger than zero as $f(r) > 1/2$,

$$\aleph_{12} = \frac{f(r)^2 - \frac{1}{4}}{4 - f(r)^2}. \quad (4)$$

The negativity of two electrons as the function of the distance of $k_F r$ at T=0 K for the spin-orbital and spin systems is shown in Fig. 1. We find that in the present spin-orbital system the quantum entanglement length r_e is about $2.4/k_F$, considerably larger than that in the spin system. Considering the shrinking of the Fermi energy in the quarter-filling spin-orbital system, the entanglement length is about 1.7 times larger than that in the spin system. In the present itinerant electron system, the two-particle spin-orbital density matrix (3) can be expressed as: $\rho = [4(1 - f(r)^2)I/16 + 3f(r)^2\rho']/(4 - f(r)^2)$, where ρ' is the density matrix composing of all spin-orbital two-particle antisymmetric states and I is the 16-order unit matrix. As a contrast, the 4-order density matrix in the spin system is $\rho_0 = [(2(1 - f(r)^2)I_0/4 + f(r)^2\rho'_0)/(2 - f(r)^2)]$, where ρ'_0 is the density matrix of spin singlet state and I_0 is the 4-component unit matrix. Evidently, the unit matrix represents completely mixed disentangled state, so the more the weight of the unit matrix in ρ is, the more disentangled the state is. At sufficient large distance $k_F r$, the weight of the unit matrix, or the disentangled component, in the spin-orbital density matrix ρ is much smaller than that in the spin density matrix ρ_0 , leading to a significantly large quantum entanglement length in the spin-orbital system.

For two particles located at the same position, their spatial wavefunctions are the same. Due to Pauli principle, the spin and orbital wavefunctions must be antisymmetric, and it does not contribute to the unit matrix. Thus the entanglement of the two electrons at is maximal at $r = 0$, as shown in Fig.1. Meanwhile, the spin-orbital wavefunction of the two electrons is composed of six antisymmetric spin-orbital substates, e.g. $|\uparrow\uparrow\rangle \otimes |\psi_\tau^- \rangle$, etc., here $|\psi_\tau^- \rangle$ is the orbital singlet state. These components are not the Bell basis wavefunctions, so ρ , though is equal to ρ' , is still a mixed-state density matrix, and the negativity is much smaller than the maximal value 1.5. Comparing to the spin system, the entanglement length and the Fermi velocity in the present system satisfy $r_e \approx 1.7r_e^0$ and $v_F = v_F^0/2^{3/4}$, respectively. Therefore, the coherent time of the entangled electrons $\tau_c \sim r_e/v_F$ is about 2.1 times larger than that of the spin system. This property is also expected to valid for the localized

electron systems. Consequently, the present system with spin and orbit DOF is more favorable than the system with only spin in the realization of quantum computation and quantum teleportation .

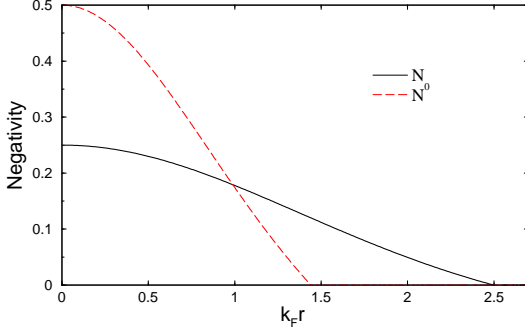


FIG. 1: Negativity as the function of spatial distance $k_F r$ of two electrons. N and N^0 represent the negativity of two electrons in the spin-orbital system and in the spin system, respectively.

It is interesting to explore the variation of the spin sub-entanglement of two electrons with the spatial distance. The reduced spin density matrix becomes,

$$\rho_{12}^s = \frac{1}{4 - f(r)^2} \left[(4 - 2f(r)^2) \frac{I_0}{4} + f(r)^2 |\psi_s^-\rangle \langle \psi_s^-| \right] \quad (5)$$

after tracing over the orbital DOF, where $|\psi_s^-\rangle$ is the spin singlet state. We find that the spin-orbital density matrix of the two electrons at the same position, $\rho_{12}^s(r=0)$, is equal to that in the spin system at the entangled distance, $\rho^0(r_e)$, indicating that even at the maximally entangled spin-orbital states, the spin of two electrons in itinerant electron system is disentangled. The vanishing spin sub-entanglement in itinerant electron systems arises from the enlargement of Hilbert state space, which greatly reduces probability of forming spin singlet state. The spin correlation functions, $\langle \mathbf{S}_i \mathbf{S}_j \rangle$, also manifest the disentanglement of the spin DOF. We find at $r=0$, $\langle \mathbf{S}_i \mathbf{S}_j \rangle = -1/4$, showing that the two electrons are classical AFM correlated. With the increase of the separation between two electrons, the classical AFM correlation becomes smaller and smaller. Therefore the spin sub-entanglement in any spin-orbital state vanishes at any distance in itinerant electron systems.

B. Entanglement and Phase Diagram in Localized Electron Systems

To explore the relationship between the variation of the entanglement and quantum phase transitions in many-electron systems, we study the entanglement in the localized spin-orbital interacting systems in what follows. Consider a one-dimensional system with strong spin-

orbital correlation [14, 15]. Its Hamiltonian reads:

$$H = \sum_i [\mathbf{S}_i \cdot \mathbf{S}_{i+1} \tau_i \cdot \tau_{i+1} + J_s \mathbf{S}_i \cdot \mathbf{S}_{i+1} + J_\tau \tau_i \cdot \tau_{i+1} + B_s S_i^z + B_\tau \tau_i^z] \quad (6)$$

where J_s and J_τ are the spin and the orbital exchange constants, respectively, and B_s (B_τ) is a small magnetic (orbital) field. In the absence of the small external fields, both the spin and the orbital parts in Eq.(6) satisfy the SU(2) symmetry, the so-called SU(2) \otimes SU(2) model. The periodic condition on Eq.(6) implies that the entanglement between arbitrary two sites is an uniform function of distance. The Hamiltonian commutes with the z-components of the total spin and the total orbital operators, $[H, S^z] = 0$ and $[H, \tau^z] = 0$, where $S^z = \sum_i S_i^z$ and $\tau^z = \sum_i \tau_i^z$. So each eigenstate of the Hamiltonian is also the eigenstate of S^z and τ^z . One can use the index (S^z, τ^z) to characterize the main four phases of this model in different regions of the exchange constants J_s and J_τ : Phase I with $(S^z=N/2, \tau^z=N/2)$, Phase II with $(N/2, 0)$, Phase III with $(0, N/2)$ and Phase IV with $(0, 0)$, as shown in Fig.2. In the present situation the spin-orbital entanglement can be explicitly expressed in terms of the spin-orbital correlation functions. Using the reduced density matrix of two nearest-neighbor particles, one can analytically express the negativity $\aleph_{[i,i+1]}$ as the nearest-neighbor spin-spin, orbital-orbital and spin-orbital correlation functions in each phase. For instance in the phase IV, the negativity reads:

$$\begin{aligned} \aleph_{[i,i+1]} = & 2|d| + |c-h| + |c+h| + |b-f| + |b+f| \\ & + \frac{1}{2} [|a-g-e+k| + |a-g+e-k| + |a+g-e-k| + |a+g+e+k| - 1]. \end{aligned} \quad (7)$$

with

$$\begin{aligned} a/b = & \langle (\frac{1}{4} + S_i^z S_{i+1}^z) (\frac{1}{4} \pm \tau_i^z \tau_{i+1}^z) \rangle \\ c/d = & \langle (\frac{1}{4} - S_i^z S_{i+1}^z) (\frac{1}{4} \pm \tau_i^z \tau_{i+1}^z) \rangle \\ e/f = & \langle (\frac{1}{4} \pm \tau_i^z \tau_{i+1}^z) (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y) \rangle \\ g/h = & \langle (\frac{1}{4} \pm S_i^z S_{i+1}^z) (\tau_i^x \tau_{i+1}^x + \tau_i^y \tau_{i+1}^y) \rangle \\ k = & \langle (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y) (\tau_i^x \tau_{i+1}^x + \tau_i^y \tau_{i+1}^y) \rangle. \end{aligned} \quad (8)$$

Obviously, in the fully polarized orbital phase III, the negativity has a simple form: $\aleph_{[i,i+1]} = -1/4 - \langle \mathbf{S}_i \mathbf{S}_{i+1} \rangle$. Similarly we obtain the negativity in the completely polarized spin phase II, $\aleph_{[i,i+1]} = -1/4 - \langle \tau_i \tau_{i+1} \rangle$. The negativity vanishes in the fully polarized spin and orbital phase I. Therefore, the direct relation between the quantum entanglement and the spin and orbital correlations in strongly correlated electronic systems is thus established, and it may provide many interesting information hidden in strongly correlated systems.

Thus one could clearly find that the variation of the entanglement closely relates to the transition of quantum phases in the present system: at the critical point of the quantum phase transition, the entanglement exhibits a discontinuous change. The entanglement phase diagram of a 4-site finite system is shown in Fig. 2. In the phase diagram Fig.2a, we adopt $\aleph_{[i,i+1]}^{s(\tau)}$ and the sub-negativity $\aleph_{[i,i+1]}^{s(\tau)}$ to characterize these different quantum phases. Very interesting, we find that the finite-

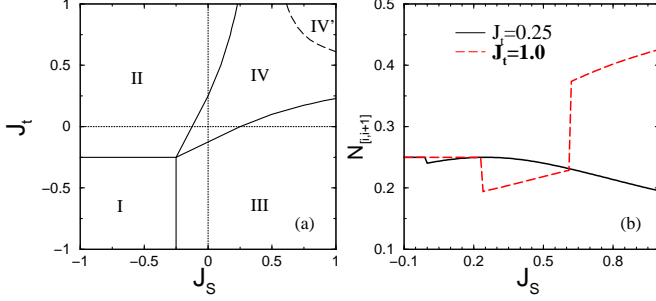


FIG. 2: Entanglement phase diagram of 4 particles in (a) and dependence of negativity on magnetic exchange constant J_s at $J_\tau = 0.25$ and $J_\tau = 1.0$ in (b). Phases I, II, III and IV represent the FM and FO state with $(S^z=2, \tau^z=2)$, the FM and AFO state with $(2,0)$, the AFM and FO state with $(0,2)$, and the AFM and AFO state with $(0,0)$, respectively. Phase IV differs from IV' in the spin-orbital correlation function, see the address in the text.

site entanglement phase diagram in Fig. 2(a) is almost identical to the magnetic and orbital phase diagram in the one-dimensional infinite lattice [14, 15], indicating that the quantum information of infinite systems manifests through the entanglement of proper finite clusters. The phase diagram in Fig.2a can also be characterized by the spin-orbital index (S^z, τ^z) . Among these phases in Fig.2a, the states in Phase I are disentangled, corresponding to fully polarized spin and orbital states with $(S^z=2, \tau^z=2)$, i.e. the ferromagnetic (FM) and ferro-orbital (FO) state. In Phase II, the negativity satisfies $\aleph_{[i,i+1]}^s = \aleph_{[i,i+1]}^\tau$ and $\aleph_{[i,i+1]}^s = 0$, indicating the states in Phase II are FM and antiferro-orbital (AFO) with $(2,0)$. Similarly, Phase III corresponds to the AFM and FO states with $(0,2)$. Both Phases IV and IV' correspond to AFM and AFO with $(0,0)$, while these two phases are distinguished by the spin-orbit correlation functions. In Phase IV, $\langle \mathbf{S}_i \cdot \mathbf{S}_{i+1} \tau_i \cdot \tau_{i+1} \rangle < 0$, and in Phase IV', $\langle \mathbf{S}_i \cdot \mathbf{S}_{i+1} \tau_i \cdot \tau_{i+1} \rangle > 0$. This difference arises from the fact that when either J_s or J_τ becomes large while the other one is small, $\langle \mathbf{S}_i \cdot \mathbf{S}_{i+1} \rangle < 0$ and $\langle \tau_i \cdot \tau_{i+1} \rangle < 0$. Due to the quantum fluctuation, $\langle \mathbf{S}_i \cdot \mathbf{S}_{i+1} \tau_i \cdot \tau_{i+1} \rangle < 0$, in Phase IV. When both J_s and J_τ become large enough, the strong AFM and AFO correlations polarize the spins and orbits, and lead the spin-orbital correlation function $\langle \mathbf{S}_i \cdot \mathbf{S}_{i+1} \tau_i \cdot \tau_{i+1} \rangle$ to transition from negative to positive, as we see the phase IV' in Fig.2a. The discontinuous

changes of entanglement of two electrons near the phase boundary are in accordance with the critical points of the quantum phase transitions, as clearly shown in Fig 2(b). At $J_s=J_\tau=1/4$ and $B_s=B_\tau=0$, the system exhibits SU(4) symmetry [17], then the ground state is highly degenerate and the negativity comes to the maximum. These results clearly demonstrate that the entanglement is closely related with the quantum phase transitions in strongly correlated systems. It is worthy of pointing out that we introduce the small magnetic and orbital fields to lift the degeneracy of Phases II and III. In the absence of these small fields the entanglement is uncertain, as discussed by Qian, et al [16].

It is interesting that the present theory is also applicable for the nuclear systems, in which the nucleons usually possess more than one DOF, such as spin, isospin, etc. According to our results for the itinerant Fermion systems, the entanglement length of the nucleons is significantly larger than one expects. We anticipate more interesting entanglement properties in the systems with multiple degrees of freedom will be uncovered in the further studies.

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